Anomalous properties of the Kronig-Penney model with compositional and structural disorder

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Abstract

We study the localization properties of the eigenstates in the Kronig-Penney model with weak compositional and structural disorder. The main result is an expression for the localization length that is valid for any kind of self- and inter-correlations of the two types of disorder. We show that the interplay between compositional and structural disorder can result in anomalous localization.

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Recently, much attention was paid to low-dimensional disordered models with long-range correlations in random potentials. Apart from the theoretical aspects, the interest on this issue has increased significantly due to the possibility of constructing random potentials with specific correlations which result in a strong enhancement or reduction of the localization length [1, 2, 3, 4, 5, 6]. These new effects allow for the fabrication of electron and optic/electromagnetic devices with desired anomalous transport properties. As was shown analytically [2, 3, 4] and confirmed experimentally [5, 6],

one can arrange prescribed windows of energy with perfect transmission (or reflection) of scattering waves.

One of the most important models, both from the theoretical and experimental point of view, is the Kronig-Penney (KP) model, which was introduced long ago to analyze electronic states in crystals [7]. Since the '80s, this model has attracted considerable attention because it provides a convenient description of superlattices (see, e.g., [8] and references therein). Modifications of the standard Kronig-Penney model have been suggested for a study of the physics of random and quasi-periodic systems with various applications, see, e.g., [9]. Recently, the Kronig-Penney model has been used to discuss the possibility of selective transmission in waveguides (see [5, 6] and references therein).

In this paper we study the KP model with two types of weak disorder. Disorder of the first kind, or "compositional", is due to small variations in strength of the delta-shaped barriers. In addition, the spacings between the barriers can be also randomly perturbed (the so-called "structural" disorder). Our interest lies in the interplay of these two kinds of disorder which can exhibit both self-correlations and mutal correlations. Our goal is to derive a formula for the localization length, and to analyze it.

The stationary Schrödinger equation for the eigenstates $\psi(x)$ has the form

$$-\frac{\hbar^2}{2m}\psi''(x) + \sum_{n=-\infty}^{\infty} U_n \delta(x - x_n)\psi(x) = E\psi(x), \tag{1}$$

where $U_n = U + u_n$ and x_n are amplitude and position of the n-th δ-barrier. In what follows we use units in which $\hbar^2/2m = 1$; we can thus write the energy of the eigenstates as $E = q^2$ where q is the electron wavenumber.

The positions of the δ-barriers are assumed to be slightly shifted with respect to the lattice sites, $x_n = na + a_n$, where a is the lattice step. The variables u_n represent fluctuations of the barrier strength around the mean value U. Our analysis is restricted to the case of weak disorder for which both variables u_n and a_n have zero average, $\langle u_n \rangle = 0$ and $\langle a_n \rangle = 0$, and small variances, $q^2\langle a_n^2 \rangle \ll 1$ and $\langle u_n^2 \rangle \ll U^2$. We remark that the condition $q^2\langle a_n^2 \rangle \ll 1$ implies that the energy must be low on a scale set by $1/\langle a_n^2 \rangle$. Note that in contrast with many previous studies, *both* variables are random and may have stationary correlations: our main interest lies in how these correlations shape the properties of the localization length $l_{\rm loc}(E)$ of the eigenstates.

It is convenient to introduce the relative displacements of the barriers, $\Delta_n = a_{n+1} - a_n$, having zero mean, $\langle \Delta_n \rangle = 0$, and small variance, $q^2 \langle \Delta_n^2 \rangle \ll 1$. Apart from the first two moments of the random variables Δ_n and u_n, one has to give the binary correlators,

$$\begin{array}{rcl} \chi_1(k) & = & \langle u_n u_{n+k} \rangle / \langle u_n^2 \rangle \\ \chi_2(k) & = & \langle \Delta_n \Delta_{n+k} \rangle / \langle \Delta_n^2 \rangle \\ \chi_3(k) & = & \langle u_n \Delta_{n+k} \rangle / \langle u_n \Delta_n \rangle . \end{array} \tag{2}$$

We will not attribute specific forms to the correlators $\chi_i(k)$; we simply assume that they depend only on the index difference k because of the spatial homogeneity in the mean of the model and that they are even functions of k.

It is worthwhile to note that Eq. (1) can be treated as the wave equation for electromagnetic waves in a one-dimensional (1D) waveguide with wavenumber $q = \omega / c$. Therefore our results are equally applicable to the classical scattering in optical and microwave devices of the Kronig-Penney type with correlated disorder. Our model is also equivalent to a classical oscillator with a parametric perturbation constituted by a succession of δ-kicks whose amplitudes and time-dependence are determined by U_n and a_n. This correspondence allows one to cast Eq. (1) in the form

$$\ddot{x} + [q^2 - \sum_{n=-\infty}^{\infty} U_n \delta\left(t - t_n\right)] x = 0. \tag{3}$$

Our analysis is based on the Hamiltonian approach [10, 11] according to which the spatial structure of eigenstates of the KP-model can be analyzed by exploring the time evolution of the kicked oscillator described by the dynamical equation (3). Such a dynamical approach considers the Schrödinger equation as an initial-value problem and can be treated as a modification of the transfer matrix approach.

Integrating the dynamical equation (3) between two successive kicks, one obtains the map

$$\begin{array}{rcl} x_{n+1} & = & \left[(U_n/q) \sin\left(\mu + \mu_n\right) + \cos\left(\mu + \mu_n\right) \right] x_n \\ & + & (1/q) \sin\left(\mu + \mu_n\right) p_n \\ p_{n+1} & = & \left[U_n \cos\left(\mu + \mu_n\right) - q \sin\left(\mu + \mu_n\right) \right] x_n \\ & + & \cos\left(\mu + \mu_n\right) p_n \end{array} \tag{4}$$

where $\mu = qa$ and $\mu_n = q\Delta_n$, and the values x_n and p_n refer to the instant before the $n-$th kick.

The evolution of the dynamical map (4) can be analyzed as follows. First, we make a weak-disorder expansion of Eq. (4), keeping only first- and second-order terms. The expansion is straightforward; the resulting equations, however, are lengthy and we omit them here. As a second step, we perform a canonical transformation $(x_n, p_n) \to (X_n, P_n)$, such that the unperturbed motion reduces to a simple rotation in the phase space of the new variables [3]. Such a trick allows one to eliminate the effect of the periodic kicks with constant amplitudes U. This can be done with the use of the canonical transformation,

$$\begin{array}{rcl} x_n & = & \alpha\cos(\mu/2)X_n + (q\alpha)^{-1}\sin(\mu/2)P_n \\ p_n & = & -q\alpha\sin(\mu/2)X_n + \alpha^{-1}\cos(\mu/2)P_n \end{array} \tag{5}$$

where the parameter α is defined by the relation

$$\alpha^4 = \frac{1}{q^2}\frac{\sin\mu - \frac{U}{2q}(\cos\mu - 1)}{\sin\mu - \frac{U}{2q}(\cos\mu + 1)}.$$

Note that, due to the transformation (5), the new variables X_n and P_n have the same dimension.

In the absence of disorder, i.e., for $u_n = 0$ and $\Delta_n = 0$, the rotation angle γ between successive kicks is determined by the relation,

$$\cos\gamma = \cos\mu + \frac{U}{2q}\sin\mu \qquad \text{with } \gamma = ka. \tag{6}$$

In terms of the Kronig-Penney model, k is the Bloch wavevector, γ is the phase shift of the wavefunction within the lattice step a, and Eq. (6) defines the band structure of the energy spectrum.

It should be pointed out that the transformation (5) is well-defined for all values of the rotation angle γ other than $\gamma = 0$ and $\gamma = \pm\pi$ for which α either vanishes or diverges. In other words, our approach fails at the center and at the edges of the first Brillouin zone, i.e., at the edges of the allowed energy bands of the KP model. However, the approach works well in every neighborhood of these critical points.

To proceed further, it is useful to pass to the action-angle variables (J_n, θ_n), with the transformation

$$X_n = \sqrt{2J_n}\sin\theta_n, \qquad P_n = \sqrt{2J_n}\cos\theta_n$$

and to represent the Hamiltonian map (4) in terms of the new variables. Leaving aside mathematical details, we give here the final expression,

$$\begin{aligned} J_{n+1} &= D_n^2 J_n \\ \theta_{n+1} &= \theta_n + \gamma - \tfrac{1}{2}\left[1 - \cos\left(2\theta_n + \gamma\right)\right] \tilde{u}_n \\ &+ \tfrac{1}{2}\left[\upsilon - \cos\left(2\theta_n + 2\gamma\right)\right] \tilde{\Delta}_n \end{aligned} \tag{7}$$

where

$$\begin{aligned} D_n^2 &= 1 + \sin\left(2\theta_n + \gamma\right) \tilde{u}_n - \sin\left(2\theta_n + 2\gamma\right) \tilde{\Delta}_n \\ &+ \tfrac{1}{2}\left[1 - \upsilon \cos\left(2\theta_n + 2\gamma\right)\right] \tilde{\Delta}_n^2 \\ &+ \tfrac{1}{2}\left[1 - \cos\left(2\theta_n + \gamma\right)\right] \tilde{u}_n^2 \\ &- \left[\cos\gamma - \cos\left(2\theta_n + 2\gamma\right)\right] \tilde{u}_n \tilde{\Delta}_n. \end{aligned} \tag{8}$$

Here, $\upsilon = \left[q\alpha^2 + (q\alpha^2)^{-1}\right] q \sin\gamma / U$, and we have introduced the rescaled random variables,

$$\tilde{u}_n = \frac{\sin\mu}{q\sin\gamma} u_n \quad \text{and} \quad \tilde{\Delta}_n = \frac{U}{\sin\gamma} \Delta_n.$$

In Eqs. (7) and (8) we have kept only the terms of the weak-disorder expansion which are necessary to compute the localization length within the second-order approximation. We remark that the angle variable evolves independently of the action variable.

The inverse localization length for the KP model (1) can be computed as the Lyapunov exponent λ,

$$l_{\text{loc}}^{-1} = \lambda = \lim_{N\to\infty} \frac{1}{Na} \sum_{n=1}^{N} \ln\left|\frac{\psi_{n+1}}{\psi_n}\right| = \left\langle \frac{1}{a} \ln\left|\frac{\psi_{n+1}}{\psi_n}\right| \right\rangle$$

which, in terms of the dynamical map (7), can be written as [11],

$$\lambda = \left\langle \frac{1}{2a} \ln\left(\frac{J_{n+1}}{J_n}\right) \right\rangle = \frac{1}{2a} \langle \ln D_n^2 \rangle. \tag{9}$$

By expanding the logarithm of D_n^2, one gets

$$\begin{aligned} \lambda &= \tfrac{1}{2a}\Big\langle \Big\{ \sin\left(2\theta_n + \gamma\right) \tilde{u}_n - \sin\left(2\theta_n + 2\gamma\right) \tilde{\Delta}_n \\ &+ \tfrac{1}{4}\left[1 - 2\upsilon \cos\left(2\theta_n + 2\gamma\right) + \cos\left(4\theta_n + 4\gamma\right)\right] \tilde{\Delta}_n^2 \\ &+ \tfrac{1}{4}\left[1 - 2\cos\left(2\theta_n + \gamma\right) + \cos\left(4\theta_n + 2\gamma\right)\right] \tilde{u}_n^2 \\ &- \tfrac{1}{2}\left[\cos\gamma - 2\cos\left(2\theta_n + 2\gamma\right) + \cos\left(4\theta_n + 3\gamma\right)\right] \tilde{u}_n \tilde{\Delta}_n \Big\} \Big\rangle. \end{aligned} \tag{10}$$

Now, in order to obtain the Lyapunov exponent λ, we have to perform the average over the phase θ_n and the random variables u_n and Δ_n. To the second order of perturbation theory, one can neglect the correlations between θ_n and the quadratic terms $\tilde{u}_n^2$, $\tilde{\Delta}_n^2$, and $\tilde{u}_n\tilde{\Delta}_n$. Hence for the summands in Eq. (10) which contain these quadratic terms, one can compute separately the averages over θ_n and over the random variables u_n and Δ_n.

In analogy with the Anderson model (see details and references in [11]), it can be shown that for our purposes it is safe to assume that the invariant measure of the phase is a flat distribution, $\rho(\theta) = 1/(2\pi)$. The assumption holds for all values of γ, except for $\gamma = \pm\pi/2$ where a small modulation of the invariant measure results in an anomaly for the localization length. The situation with these values of γ is similar to that known for the standard 1D Anderson model at the center of the energy band, and the correct expression for λ can be obtained following the approach of [11].

It should be stressed that weak modulations of $\rho(\theta)$ arise also for other "resonant" values, $\gamma = m\pi/r$, with m and r integers prime with each other and $r > 2$. However, these modulations do not influence the value of λ, because the expression to be averaged in Eq. (10) has no harmonics higher than 4θ. Thus, our further analysis is valid for all values of γ except $\gamma = 0$ and $\gamma = \pm\pi$ (i.e., the edges of the energy bands) and $\gamma = \pm\pi/2$.

After averaging, the expression for the Lyapunov exponent takes the form,

$$\begin{aligned} \lambda &= \frac{1}{8a}\left[\langle\tilde{u}_n^2\rangle + \langle\tilde{\Delta}_n^2\rangle - 2\langle\tilde{u}_n\tilde{\Delta}_n\rangle\cos\gamma\right] \\ &+ \frac{1}{2a}\langle\tilde{u}_n\sin(2\theta_n+\gamma)\rangle - \frac{1}{2a}\langle\tilde{\Delta}_n\sin\left(2\theta_n+2\gamma\right)\rangle. \end{aligned} \tag{11}$$

In order to compute the noise-angle correlators in Eq. (11), we generalize the method used in [2]. Specifically, we introduce the correlators $r_k = \langle\tilde{u}_n\exp\left(i2\theta_{n-k}\right)\rangle$ and $s_k = \langle\tilde{\Delta}_n\exp\left(i2\theta_{n-k}\right)\rangle$. Both correlators satisfy recursive relations that can be obtained by substituting the angular map of Eq. (7) into the definitions of r_{k-1} and s_{k-1}. The recursive relations allow one to obtain the correlators r_0 and s_0, whose imaginary parts represent the noise-angle correlators in Eq. (11). As a result, we arrive at the final

expression for the Lyapunov exponent,

$$\begin{aligned}
\lambda &= \frac{1}{8a}\left[\langle\tilde{u}_n^2\rangle W_1 + \langle\tilde{\Delta}_n^2\rangle W_2 - 2\langle\tilde{u}_n\tilde{\Delta}_n\rangle \cos\gamma W_3\right] \\
&= \frac{\sin^2\mu}{8aq^2\sin^2\gamma}\langle u_n^2\rangle W_1 + \frac{U^2}{8a\sin^2\gamma}\langle\Delta_n^2\rangle W_2 \\
&- \frac{1}{4a}\frac{U\sin\mu}{q\sin^2\gamma}\cos\gamma\ \langle u_n\Delta_n\rangle W_3
\end{aligned} \tag{12}$$

where the functions

$$W_i \equiv W_i\,(2\gamma) = 1 + 2\sum_{k=1}^{\infty}\chi_i(k)\cos(2\gamma k) \quad (i = 1, 2, 3) \tag{13}$$

are the $2\gamma-$harmonics of the Fourier transform of the binary correlators $\chi_i(k)$, see Eq. (2). We should stress that Eq. (12) has been derived without invoking the Born approximation, $E \gg U$; it describes the tunneling regime for $E < U$ as well as the scattering one, $E > U$. The only constraint is the weakness of both types of disorder, $\langle u_n^2\rangle \ll U^2$ and $q^2\langle\Delta_n^2\rangle \ll a^2$.

Let us first discuss the structure of expression (12) for the case in which there are no correlations between u_n and Δ_n. It is quite instructive that for weak scattering, $U \ll q$, (therefore, $\gamma \approx \mu$) with purely compositional disorder, (i.e., $\Delta_n = 0$), the Lyapunov exponent takes the form $\lambda \approx \frac{\langle u_n^2\rangle}{8aq^2}W_1$, (see [6]). This is equivalent to the well-known result for weak scattering in continuous 1D potentials, $\lambda = \frac{\langle V^2\rangle}{8q^2}W(2q)$, where $\langle V^2\rangle$ is the variance of the random potential and $W(2q)$ is the $2q-$component of the power spectrum of the potential.

In the other limit case of structural disorder (i.e., $u_n = 0$), the expression for the Lyapunov exponent, $\lambda = \frac{U^2}{8a\sin^2\gamma}\langle\Delta_n^2\rangle W_2$, was obtained in [3]. One can see that it is similar to the expression for the tight-binding Anderson model with diagonal disorder, $\lambda = \frac{\langle\varepsilon^2\rangle}{8a\sin^2\mu}W(2\mu)$, where $\langle\varepsilon^2\rangle$ is the variance of the random site-potential, μ is the phase shift of the wavefunction between two sites -related to the energy by the dispersion relation $E = 2\cos\mu$-, and $W(2\mu)$ has the same meaning as W_1.

Expression (12) for the inverse localization length allows one to estimate the relative importance of the structural and compositional disorder for the transport properties of a finite sample. As can be seen, spatial correlations of the variables u_n and Δ_n can enhance or suppress the localization length in comparison with the case of uncorrelated disorder.

Specific long-range correlations can make the Fourier transforms (13) vanish in prescribed energy windows, so that the Lyapunov exponent (12) also vanishes in the same energy intervals. A method for the construction of random potentials with given binary correlators $\chi_i(k)$ was described and tested in [2, 4]. Following the same approach, one can use formula (12) as a starting point for the fabrication of devices with prescribed anomalous transport characteristics.

It is interesting to relate the properties of the KP model with known results for 1D tight-binding models with both diagonal and off-diagonal disorder. It can be shown that, after eliminating the momenta p_n from the map (4), one obtains the equation

$$\begin{aligned} &[1/\sin(\mu+\mu_n)]\,\psi_{n+1} + [1/\sin(\mu+\mu_{n-1})]\,\psi_{n-1} \\ &= \left[\cot(\mu+\mu_n) + \cot(\mu+\mu_{n-1}) + \tfrac{1}{q}\left(U+u_n\right)\right]\psi_n \end{aligned} \tag{14}$$

where $\psi_n \equiv x_n$. For weak disorder one can expand the coefficients of Eq. (14) in powers of $q\Delta_n$ and get

$$\begin{aligned} & \left[1 + q^2\left(1/2 + \cot^2\mu\right)\langle\Delta_n^2\rangle - q\Delta_n\cot\mu\right]\psi_{n+1} \\ + & \left[1 + q^2\left(1/2 + \cot^2\mu\right)\langle\Delta_n^2\rangle - q\Delta_{n-1}\cot\mu\right]\psi_{n-1} \\ = & \Big[2\cos\mu + U\tfrac{\sin\mu}{q} + 2q^2\tfrac{\cos\mu}{\sin^2\mu}\langle\Delta_n^2\rangle \\ - & \tfrac{q}{\sin\mu}\left(\Delta_n + \Delta_{n-1}\right) + \tfrac{\sin\mu}{q}u_n\Big]\psi_n. \end{aligned} \tag{15}$$

One can see that the right-hand side of this relation vanishes under the conditions

$$U = -\frac{2q\cos\mu}{\sin\mu}\left[1 + \frac{q^2}{\sin^2\mu}\langle\Delta_n^2\rangle\right], \tag{16}$$

$$u_n = \frac{q^2}{\sin^2\mu}\left(\Delta_n + \Delta_{n-1}\right). \tag{17}$$

The first condition determines the energy as a function of the mean field U and of the variance $\langle\Delta_n^2\rangle$. The second condition establishes non-trivial correlations between the compositional and structural disorders. Under these conditions Eq. (15) reduces to

$$\begin{aligned} &\left[1 + q^2\left(1/2 + \cot^2\mu\right)\langle\Delta_n^2\rangle - q\Delta_n\cot\mu\right]\psi_{n+1} \\ &+ \left[1 + q^2\left(1/2 + \cot^2\mu\right)\langle\Delta_n^2\rangle - q\Delta_{n-1}\cot\mu\right]\psi_{n-1} = 0 \end{aligned} \tag{18}$$

and this identity can be written as the Schrödinger equation

$$(\gamma + \gamma_{n+1})\,\psi_{n+1} + (\gamma + \gamma_n)\,\psi_{n-1} = 0 \tag{19}$$

for the Anderson model with purely off-diagonal disorder at the center of the energy band.

As is known [12], the model (19) exhibits anomalous localization. Specifically, the band-center electronic state is localized but decays away from the localization center n_0 as $\psi_n \sim \exp\left(-A\sqrt{|n-n_0|}\right)$ where A is some constant. Thus, the interplay between compositional and structural disorder can give rise to anomalous localization in the KP-model.

We have to note that the above conclusion about the anomalous localization cannot be drawn directly from the general formula (12) for two reasons. First, the zero-value of the Lyapunov exponent leaves open the question of whether the corresponding electronic state is extended or anomalously localized. Second, the conditions (16) and (17) imply that the Bloch vector k lies in a neighborhood of the points $\pm\pi/2a$, where our derivation of the Lyapunov exponent may be invalid. Indeed, when conditions (16) and (17) are met, the requirement of weak compositional disorder, $\langle u_n^2\rangle \ll U^2$, leads to $q^2\langle\Delta_n^2\rangle \ll \sin^2\mu$. Taking into account this inequality and the relation (6) with U given by (16), one can see that the Bloch wavenumber is actually close to the resonant values $\pm\pi/2a$.

In conclusion, we have derived the expression for the localization length in the KP model for the general case when both the amplitudes and the spacings of the δ-barriers are random variables. Our consideration takes into account correlations of each type of disorder with itself, as well as correlations between the two disorders. The obtained expression depends on the binary correlators only and thus opens the way to the construction of random potentials with desired characteristics of the electron (or electromagnetic waves) transmission through finite samples. The most important application of expression (12) lies in its use for the fabrication of devices with prescribed energy windows with perfect transmission (or reflection) produced by long-range correlations of the disorder, an effect recently observed experimentally in microwave waveguides [5, 6]. We have also found that for specific correlations between the two kinds of disorder, the Kronig-Penney model has anomalously localized eigenstates, similarly to the Anderson model with off-diagonal disorder.

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